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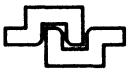

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Functional Gradient Materials and Surface Layers Prepared by Fine Particles Technology

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MD SIMULATION OF THE ION-STIMULATED PROCESSES IN SI SURFACE LAYERS

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1. Introduction

The progress in understanding of Si (001) surface structure has been well described in a series of review papers and conference proceedings [1,2] This surface has two dangling bonds per surface atom which move towards each other in pairs leading to (2x1) unit cell formation. Higher-order periodicities have been observed as well as disordered atomic configurations. Ab initio theoretical calculations of relaxation processes in semiconductor surface layers are limited by the great complexity of the phenomena involved, and thus forcing the use of simulation tools.

The Molecular Dynamics (MD) method gives a useful insight into the problem. Many results (for example [3]) show that the MD method can provide an important guide for the exploring models for Si surface, and what's more the simulation scheme may be optimized by simultaneous electronic calculations [4].

A widespread technological process in microelectronics is radiation treatment of Si surface. This process is used for surface cleaning and ion-assisted dry etching, but it has the inherent drawback that the particle – surface interaction produces a distorted and disordered surface layers. It is of great interest to study destruction and relaxation processes induced by low-energy ion bombardment of Si surface, in particular by self-ion implantation [5]. According to the ion energy dose, dose rate, and the temperature conditions Si surface can be damaged, amorphized, recrystallized [6], etc.

The problem is to clarify the conditions of the ion irradiation and to determine parameters of ion beams which stimulate relaxation processes leading to the best surface characteristics.

In this paper we described calculations of relaxation processes of Si surface layers at elevated temperatures and caused by ion beam bombardment. New details in microstructure of relaxed Si surface layers are obtained. The energy dependencies of ion-stimulated atomic processes show that the most expressed effect of improvement of Si surface layers takes place in vicinity of the energy threshold for elastic atom displacement in Si lattice.

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2. Model and Method

The starting configuration was taken as a parallelepiped containing 864 atoms: 12 layers with 72 atoms in each one. Periodic boundary conditions were used in two dimensions.

At first all atoms were in normal lattice positions. MD method was applied in its standard form [7] i.e. the equations of motion were solved by using the central difference scheme. The time-step was 10^{-14} s.

Simulations were performed with Stillinger-Weber(SW) [8] potential. Many other potentials for Si exist in the literature. But experience with SW potential indicates that it is a reasonable presentation of Si for the study of ion beam processing, accurately describing many properties of small Si clusters, bulk and surfaces.

The scenario of pulse ion irradiation was as follows. After equilibration of the system, one atom is given the velocity corresponding to the chosen energy and beam angle of incidence that needs to be simulated. Then we were waiting when the system reaches the equilibrium with the surrounding thermal bath. In the case of continuous ion irradiation the next ion pulse was done immediately after the previous one.

We have chosen new routes to investigate relaxation processes in Si surface layers. In this work we have used the new MD approach for investigations of full Si surface relaxation with taking into account the possibility of re-building and re-hybridization of chemical bonds as it was done in [9]. This approach allowed us to get new structural peculiarities of the relaxed Si surface layers.

3. Results

3.1. QUASI-DISORDERED PHASE

The results of computer simulation of Si surface relaxation processes have shown that a quasi-disordered phase (QDP) arises as a result of free Si surface relaxation. Only four near-surface layers form the QDP. The model has emphasized that in particular the microstructural constituents in relaxed Si surface layers are nodes with one or more dangling bonds. One can see that the Radial Distribution Functions and Angle Distribution Functions (the angles between chemical bonds are implied) are similar to those for a-Si (Fig.1). As a result of relaxation non-hexagonal polygons and dangling bonds were discovered in Si near-surface layers. The fifth layer does not differ practically from more deep layers.

Each of four layers which forms the QDF has his specific structural characteristics. The third layer has less structural and electronic defects in comparison with other layers of QDP. This layer almost has not dangling bonds. But at the same time the third layer is the most distorted one. Atoms of the third layer are characterized by the largest displacements upwards relatively to the normal position of the corresponding crystallographic plane. Analysis of microstructure of near-surface layers of Si indicates that the third layer plays a special role in stabilization of QDP. This layer is a transitional one between the crystal volume and the surface layers.

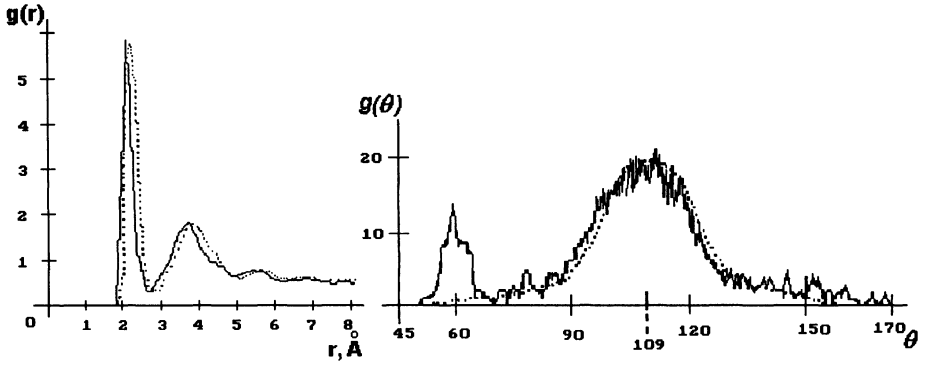

Figure 1. The Atomic Radial Distribution Function (left) and the Angle Distribution Function (right) for the relaxed (001) Si surface layers (unbroken curve). The doted lines correspond to a-Si.

3.2. STRUCTURE OF DIMERS IN RELAXED SI (001) SURFACE

Because of the structure of relaxed Si surface layers contains dangling bonds, the conditions arise for formation of dimers not only in the first layer. In near surface layers new space configurations of dimers were obtained.

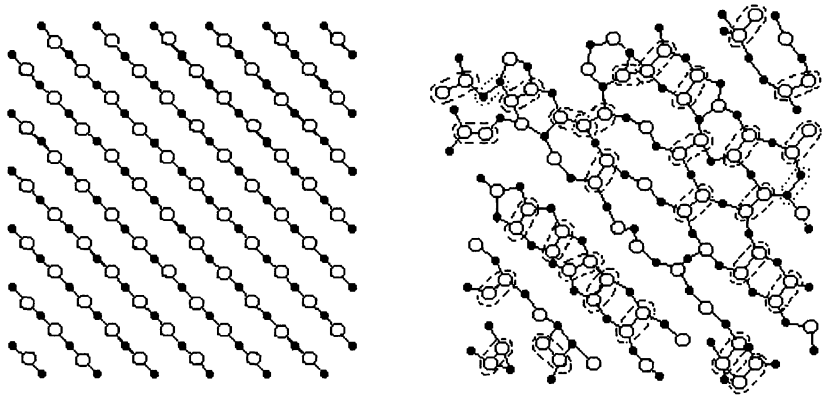

Figure 2. The dimer structure in the relaxed (001) Si surface layers (dimers in the first layer on the right). On the left is a nonrelaxed surface.

As a rule dimers are investigated by moving only atoms of the first layer by equal and opposite distances along the given direction. By using the simulation

technique which gives a full relaxation of the system and rehybridization of chemical bonds we obtained new dimer configurations besides those which are described in known works (for example, [10]).We have discovered dimers not only in the first layer and have observed their specific space orientations and size dispersion (Fig. 2).

It was established that in the second and in the third layers there is a large part of dimers which dispose under large angles of inclination to the (001) plane. In the forth layer there are few dimers, and they almost all dispose in the (001) plane. In the first layer the most of dimers is situated in vicinity of direction $\vec{d}_0$ ($\vec{d}_0$ shows the direction of ideal dimers [3].

3.3. RADIATION TREATMENT OF SI SURFACE

We investigated radiation effects in Si surface layers caused by low-energy ion bombardment. The results were obtained for the transfered energies near the threshold E_d for atom displacements in Si lattice under the elastic collisions [11]. The following energies of bombarding particles were chosen: 10, 20, 30, 40 and 50eV. The irradiation flux was modeled so that one pulse corresponded to $2 \cdot 10^{12}$ particles/sm^2·s.

For monoenergetic monoisotopic ion bombardment the induced structural changes depend on the bombardment angle. Therefore we have compared the results for different energies of ion beams at the same bombardment angles, ion doses and dose rates.

There are structural processes in this energy region of E_d which are known as "grasshopper effect" in diamond-like lattices [12]. It was shown in [12] that the displacement of atoms in Si lattice in the (111) direction under the transfered energy $E \cong E_d$ leads to arising of metastable atom configuration with unbroken chemical bonds. The relaxation of such configuration provides its displacement on whole and stimulate a migration of defects and a recovery of disordered regions.

We obtained a specific energy dependence of radiation-stimulated relaxation processes. Just it was established that the ion irradiation of Si surface in vicinity of E_d leads to the best structural characteristics of near surface layers. In Fig. 3a one can see the energy dependence of parameter ΔE, which characterizes the level of relaxation. This parameter gives a relative difference between the full energies for the initial state of the system and the state after final relaxation. The largest value of ΔE corresponds to the transfered energy $E \sim E_d$. Fig. 3b shows the energy dependence of the relaxation time. For this parameter the optimum energy also lies in vicinity of E_d.

Thus it was established that ion bombardment of Si surface in the energy region of the threshold of elastic displacement of atoms in Si lattice allows to improve structural characteristics of surface layers and decrease the relaxation time. The Fig.4a,b illustrates the influence of ion-beam treatment of Si surface on the each of near-surface layers separately and the results concerning the pulse and the continuous irradiation.

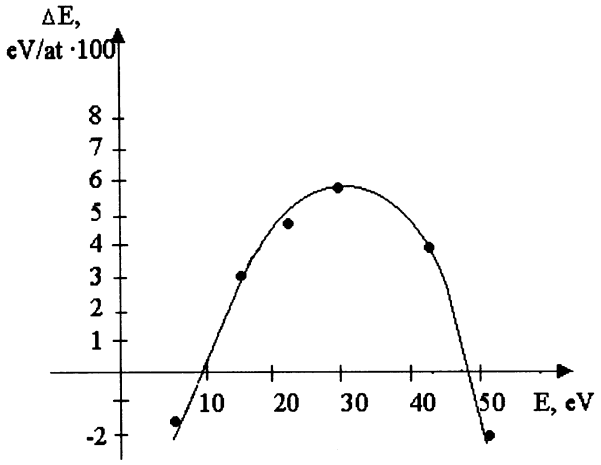

Figure 3a. Energy dependence of the level of relaxation for the pulse ion treatment of Si surface layers.

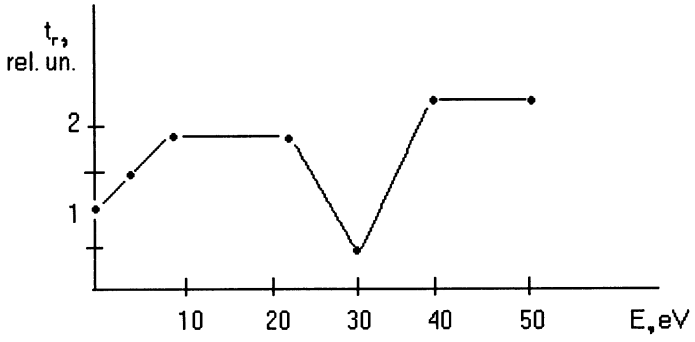

Figure 3b. Energy dependence of the relaxation time for the pulse ion of Si surface layers.

4. Conclusion

Molecular Dynamics technique gives a useful insight into the problem of radiation-stimulated semiconductor surface relaxation.

The high-temperature relaxation of the free Si surface leads to formation of quasi-disordered phase (QDP). Re-building and re-hybridization of chemical bonds may occur in the first four layers.

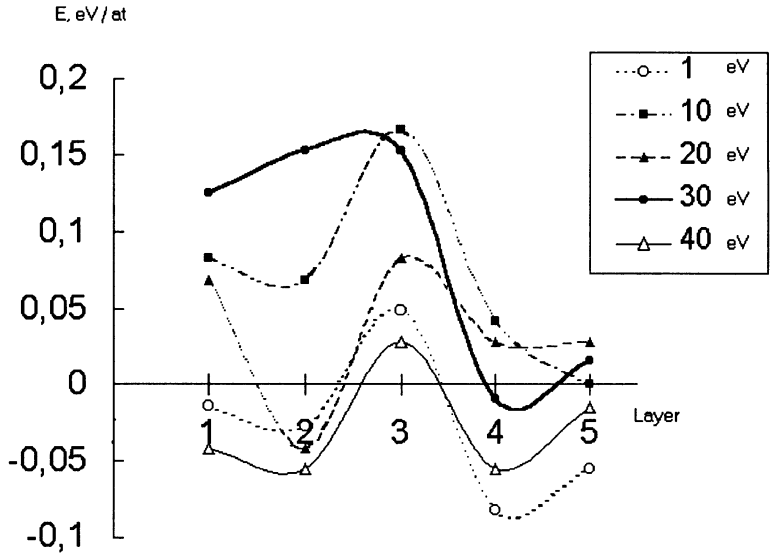

Figure 4a. Effect of radiation-stimulated restoration of different Si surface layers.

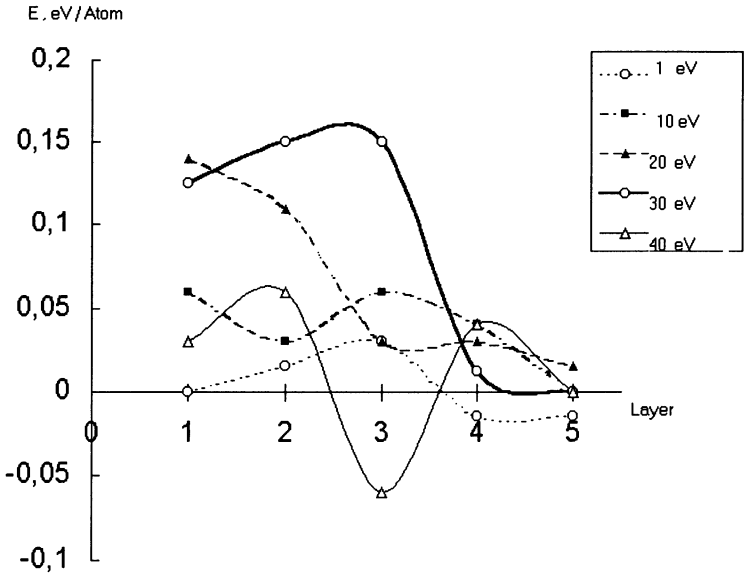

Figure 4b. Pulse treatment

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